Development and Benchmarking of a new Kinetic Code for Parallel Plasma Transport in the SOL and Divertor

A.V.Chankin[1], D.P.Coster[1], G.Meisl[1,2]

[1]*Max-Planck-Institute for Plasma Physics, Garching, Germany*
[2]*Physics Department of Munich Technical University, Germany*

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Outline

- Introduction: basics features of the code

- Coulomb collision operator, E-field force

- Code tests for 0d2v problems

- Parallel heat conduction calculations

- Summary and outlook

Basic features of KIPP: KInetic code for Plasma Periphery

- Basic version: only parallel electron kinetics. Emphasis on parallel heat flux $q_{e||}$.
  Justification: $\chi_{e||} >> \chi_{i||}$, + other reasons… Fluid equations for ions (kinetic – later).

- 1D+ structure. Solves along field lines (now), later - exchange (particle, heat) between flux surfaces. May use SOLPS grid.

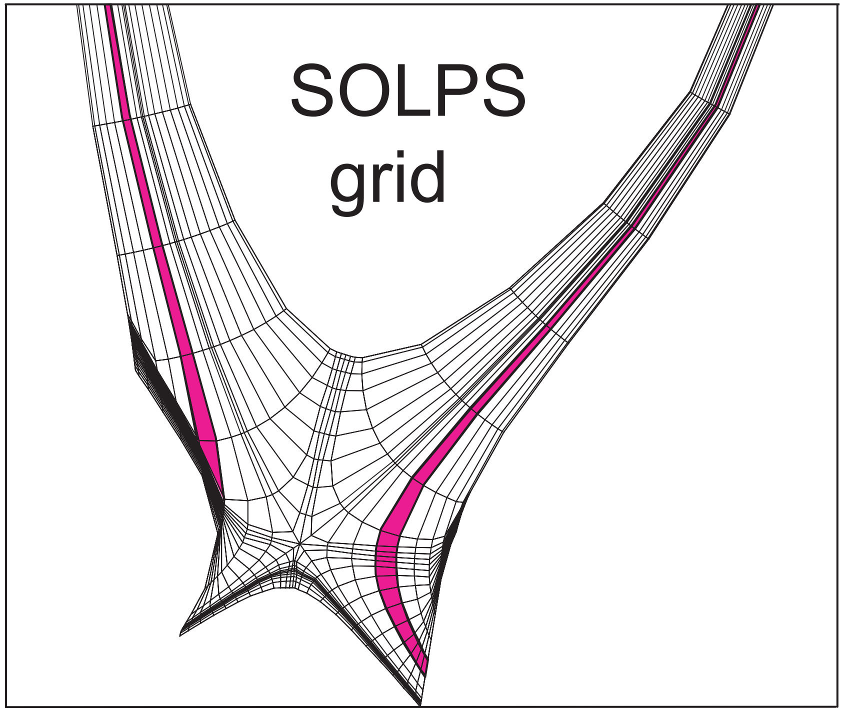
- Perpendicular (radial) transport: standard B2 treatment using ad-hock transport coefficients $\chi_{e\perp}$, $\chi_{i\perp}$, $D_\perp$, viscosity etc. (drifts – later; but No ion orbits ! (2D effect)).

- Continuum Fokker-Planck code, 1D2V ($v_{||}$,$v_\perp$)

- Plasma quasi-neutrality assumed, electron equilibrium along B achieved by adjusting $E_{||}$;
  Debye sheath not resolved, “logical sheath condition” at divertor targets

- Main ions, impurities, interaction with neutrals, plasma-wall interaction:

  to be handled by SOLPS (Eirene + B2)



ASDEX Upgrade

Ultimate goal: code integration into SOLPS as a module

IPP

- Strategy of kinetics' implementation: build up on available "infrastructure": preserve integrity of SOLPS by giving it essential control over conservation laws, plasma-neutral interaction etc.
- Kinetic module $\rightarrow$ SOLPS(B2): realistic $\chi_{e||}$, thermoforce coeff., target heat γ_e, ionization/excitation coeff. (use full distribution function f_e at every step!)

F For predicting divertor conditions in next step devices, introducing kinetics is EQUALLY IMPORTANT as preserving State of The Art description of neutrals (Eirene) and other advanced features of SOLPS $\Rightarrow$ kinetics should rather be *blended* into the existing code.

Fokker-Planck equation

$$\frac{\partial f_e}{\partial t} + v_{\|}\left(\frac{\partial f_e}{\partial s_{//}}\right) + \frac{q_e E_{\|}}{m_e}\left(\frac{\partial f_e}{\partial v_{\|}}\right) = \left(\frac{\partial f_e}{\partial t}\right)_{\mathrm{coll.}} + \text{sources}$$

- Two velocity variables: $v_{\|}$ and $v_{\perp}$ - gyro-averaged
- one spatial variable: $s_{||}$

Fokker-Planck equation (cont.)

Work in dimensionless parameters:

$$\tilde{v}_{\parallel} = \frac{v_{\parallel}}{v_o}, \quad \tilde{v}_{\perp} = \frac{v_{\perp}}{v_o}, \quad \text{where} \quad v_o = \sqrt{T_e/m_e} \quad (\text{also} \quad \tilde{w} = \frac{v_{\perp}^2}{2\,v_o^2} \quad \text{is} \quad \text{used})$$

$$\tilde{t} = \frac{t}{\tau_o}, \quad \text{where} \quad \tau_o = \frac{4\pi v_o^3}{n_o \Lambda_o}\left(\frac{4\pi e^2}{m_e}\right)^{-2} - \text{Trubnikov's "simplest relaxation time"},$$

$$\tilde{s}_{\parallel} = \frac{s_{\parallel}}{v_o \tau_o},$$

$$\tilde{E} = \frac{E_{\parallel}}{E_o}, \quad E_o = \frac{m_e v_o^2}{q_e \tau_o},$$

$$\tilde{f} = f\,\frac{v_o^3}{n_o}$$

Fokker-Planck equation (cont.)

In dimensionless parameters:

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{v}_{\|}\left(\frac{\partial \tilde{f}}{\partial \tilde{s}_{\|}}\right) - \tilde{E}_{\|}\left(\frac{\partial \tilde{f}}{\partial \tilde{v}_{\|}}\right) = \left(\frac{\partial \tilde{f}}{\partial \tilde{t}}\right)_{\text{coll.}}$$

- Operator-splitting scheme used to separate contributions to $\frac{\partial \tilde{f}}{\partial \tilde{t}}$ from:

  - $\tilde{v}_{\|}\left(\frac{\partial \tilde{f}}{\partial \tilde{s}_{\|}}\right)$ "free-streaming"

  - $-\tilde{E}_{\|}\left(\frac{\partial \tilde{f}}{\partial \tilde{v}_{\|}}\right)$ parallel E-field force

  - $\left(\frac{\partial \tilde{f}}{\partial \tilde{t}}\right)_{\text{coll.}}$ Coulomb collisions

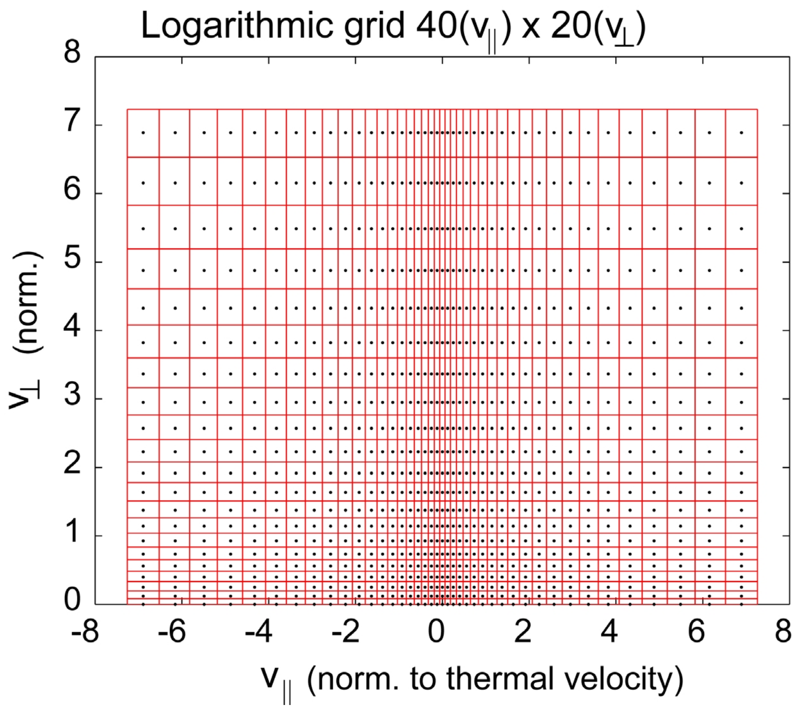
These two can be easily combined in one implicit scheme (see later)

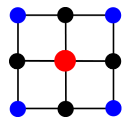
Full non-linear Coulomb collision operator

$$\frac{\partial\tilde{f}}{\partial t}=\tilde{C}(\tilde{f})=-\frac{\partial\tilde{\Gamma}_{\tilde{v}_\parallel}}{\partial\tilde{v}_\parallel}-\frac{1}{\tilde{v}_\perp}\frac{\partial\tilde{\Gamma}_{\tilde{v}_\perp}}{\partial\tilde{v}_\perp},\quad \text{where}\begin{cases}\tilde{\Gamma}_{\tilde{v}_\parallel}=-\tilde{D}_{\tilde{v}_\parallel}\tilde{f}-\tilde{D}_{\tilde{v}_\parallel\tilde{v}_\parallel}\dfrac{\partial\tilde{f}}{\partial\tilde{v}_\parallel}-\tilde{D}_{\tilde{v}_\parallel\tilde{v}_\perp}\dfrac{\partial\tilde{f}}{\partial\tilde{v}_\perp}\\ \tilde{\Gamma}_{\tilde{v}_\perp}=-\tilde{D}_{\tilde{v}_\perp}\tilde{f}-\tilde{D}_{\tilde{v}_\perp\tilde{v}_\parallel}\dfrac{\partial\tilde{f}}{\partial\tilde{v}_\parallel}-\tilde{D}_{\tilde{v}_\perp\tilde{v}_\perp}\dfrac{\partial\tilde{f}}{\partial\tilde{v}_\perp}\end{cases}$$

D-coeff. are found by calculating Rosenbluth potentials and their derivatives

“dynamic friction” | pitch-angle scattering | diffusion



- Logarithmic mesh in $v_\parallel$, $v_\perp$ space to fit wide range of T_e’s
- 9-point stencil discretization scheme 
- Implicit solution using MUMPS sparse matrix solver for both Fokker-Planck eq. and two Rosenbluth potentials (Poisson eqs. on 5-pt stencil) $\Rightarrow$ MUMPS is used 3 times on each time step

Tests for 0d2v problems (one spatial position)

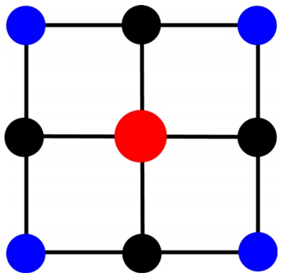
- Maxwellian (also shifted along $v_{||}$) can be well maintained; initial non-Maxwellian distribution relaxes to a Maxwellian; no instabilities seen

- Slow energy drift (loss of energy content due to energy non-conservation in e-e collisions); reduces linearly with increase in the number of velocity grid cells (mmax^2) $\rightarrow$ 2nd order scheme

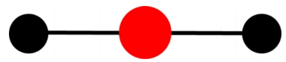
- Excellent match with Spitzer electrical conductivity for small $E_{||}$ and theoretical e-i energy equipartition rate (see later)

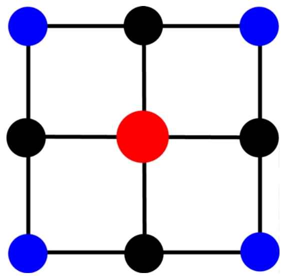
Plasma electrical conductivity: fast convergence scheme

9-pt stencil for Coulomb collisions



3-pt stencil for E-field action
(1st order upwind scheme)





can be easily combined in a
common implicit scheme

F During tests on electrical conductivity and runaway electron rate on typical grids in use, performance of the combined scheme was found to be of 2nd order (error $\propto$ *mmax*^2), despite E-field action is described by only 1st order scheme

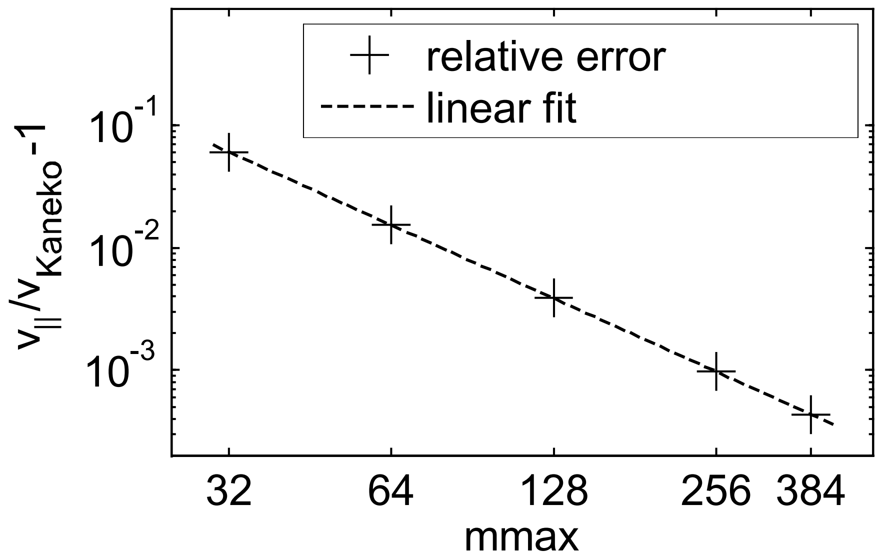
Electrical conductivity tests

- $\tilde{E} = -0.002$, $\approx$ 1% of Dreicer's field
- uniform velocity grid; v_{max} = 10 thermal velocities
- 130 time steps of τ_{ei}
- full non-linear coll. operator for e-e coll., linear coll. operator – for e-i coll.

Electron velocity $v_{e||}=-j_{||}/en$, in dimensionless parameters: $\tilde{v}_{\|} = K \dfrac{\tilde{T}_e^{3/2}}{\tilde{\Lambda}_c \tilde{n}_e} \tilde{E}$

K = 7.37 – Braginskii
7.343 - Balescu
7.425 – Spitzer
7.425886 - Kaneko (1978)

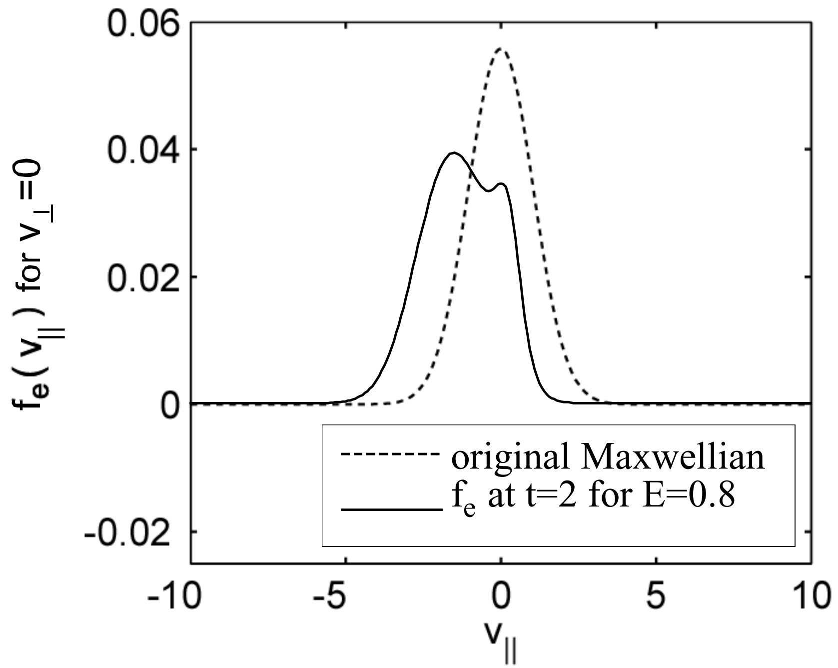
Relative error vs. Kaneko's result



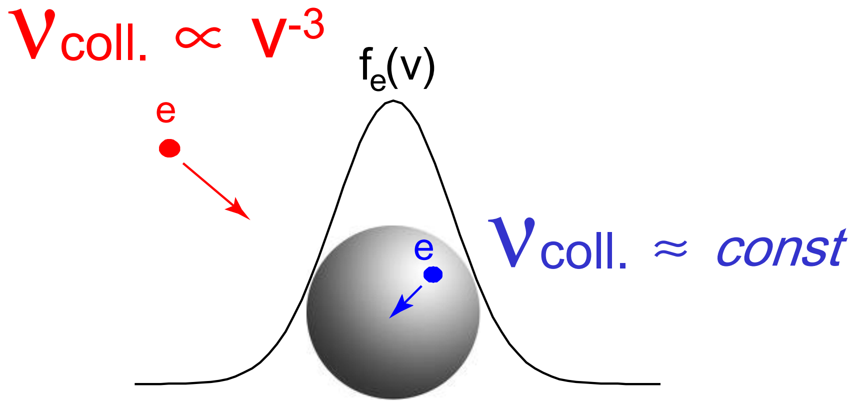
- Good convergence to best available results on electrical conductivity with improving grid resolution

Electrical conductivity tests (cont.)

- Subtle feature of doubly peaked f_e-function (extra peak – near $v_{\|}=0$, where ions sit) at large $\tilde{E}_{\|}=0.8$ (4×Dreicer's field) after $\Delta t = 2\tau_{ei}$



- Ion velocities << electron velocities ⇒ collision frequency for e-i collisions scales as v^-3 down to very small values of v; Extremely high e-i coll. rate for low energy → electrons "attemp" to create a local Maxwellian around ion velocities



e-i energy equipartition (deuterium ions)

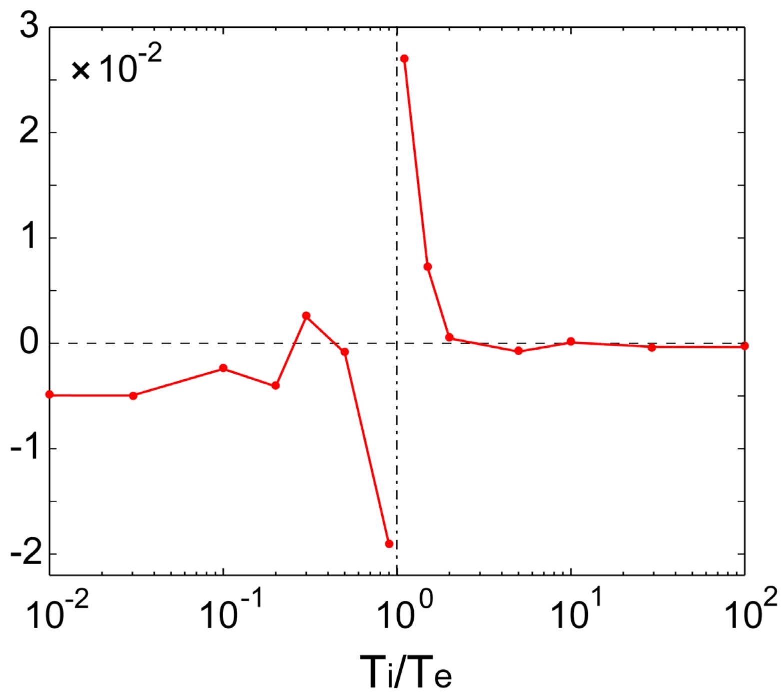
- Uniform velocity grid with v_{max}=10 electron thermal velocities, 400 cells in $v_{||}$ ($-10v_{th}$ to $+10v_{th}$) and 200 cells in $v_{\perp}$ (400x200 grid)
- Full non-linear Coulomb coll. operator for e-e collisions & linear coll. operator for e-i collisions
- Initial Maxwellian distributions for ions and electrons

Relative deviation from Trubnikov's formula for $\Delta t=10^{-9}\,\tau_o$ for different T_i/T_e ratios

(τ_o – Trubnikov's "basic relaxation time", used for thermal electrons with $v_e=\sqrt{(T_e/m_e)}$ colliding with species of mass $\rightarrow$ ¥)

▶ Satisfactory agreement with theory

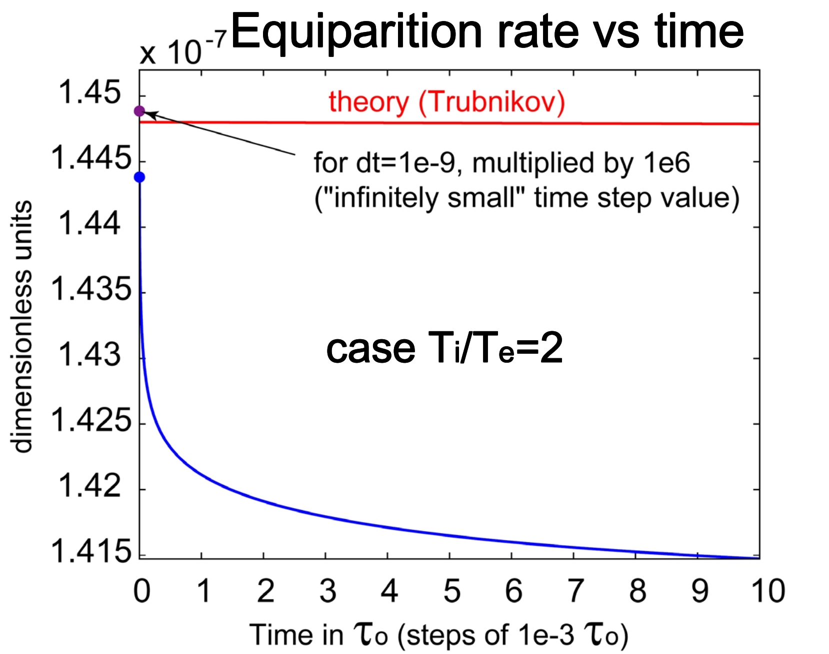
$$\left(\frac{dT_e}{dt}\Big|_{code} - \frac{dT_e}{dt}\Big|_{theory} \right) \Big/ \frac{dT_e}{dt}\Big|_{theory}$$



e-i energy equipartition (cont.)

- Excellent agreement with theory for (initially) Maxwellian f_e and f_i. and smallest time step. However, equipartition rate drops by 2.3% over $10\tau_o$ (e-i coll. times) compared to theory value, in line with theoretical expectations of large f_e – distortion at very low electron energies ~ Ti/400 (*Trubnikov, 1965*):

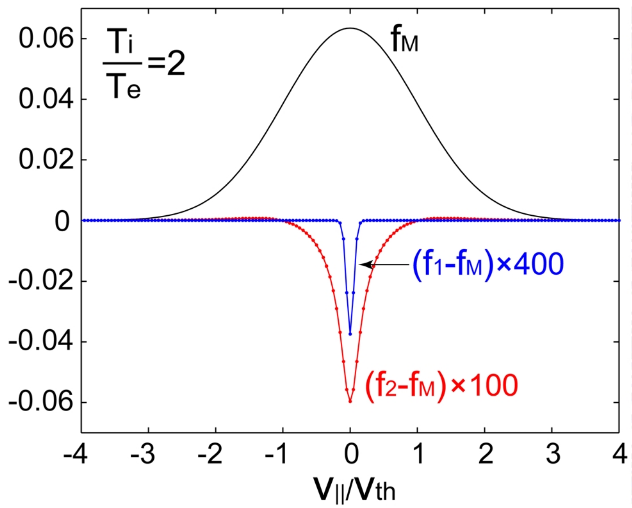
$$\frac{d\varepsilon_\alpha}{dt} = -\frac{2\varepsilon_\alpha}{\tau_1^{\alpha/\beta}(\varepsilon_\alpha)}\left[\frac{m_\alpha}{m_\beta}\mu(x_\beta) - \mu'(x_\beta)\right]$$, where $\varepsilon_\alpha = \frac{m_\alpha v_\alpha^2}{2}$

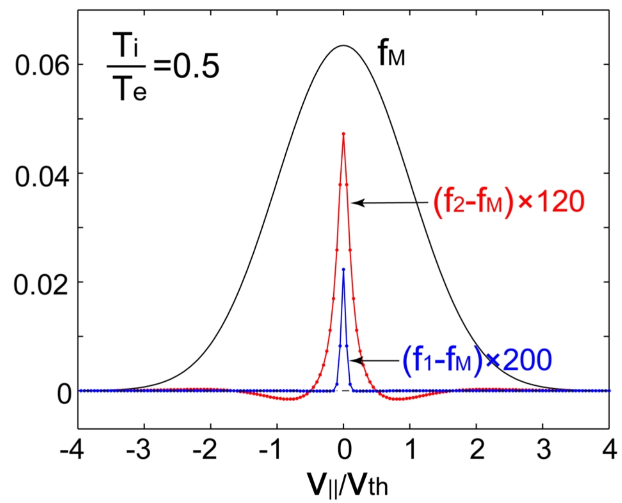


- Fine structure of f_e during energy equipartition with ions can be resolved by the code

-f_1 – f_e after $10^{-3}\times\tau_o$

- f_2 – f_e after $1\times\tau_o$
- f_M - Maxwellian
- all f's – for $v_\perp=0$





Parallel heat conduction calculations

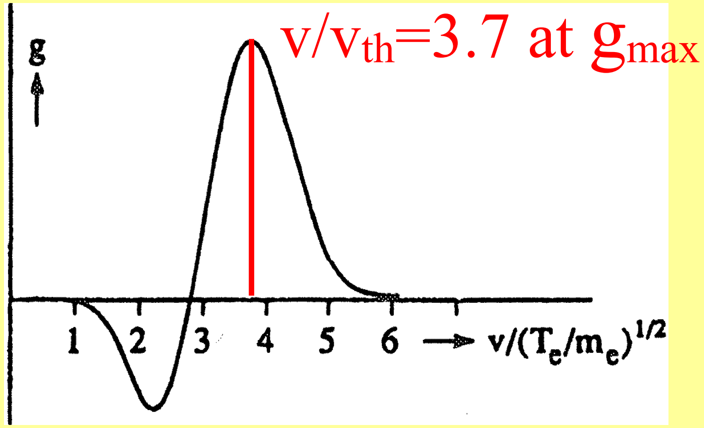
- **Main challenge**: classical (Spitzer-Härm/Braginskii) parallel heat conduction is determined by supra thermal particles, e.g., for electrons: $v_e = 3-5\sqrt{T_e/m_e}$ their collisionality is dramatically reduced:

$$\frac{L_{\text{mfp-fast}}}{L_{\text{mfp-thermal}}} \approx \frac{(3.7^\wedge 2/2T_e + 1T_e)^{3/2}}{(3/2T_e)^{3/2}} \times \frac{3.7 v_{e,th}}{v_{e,th}} \approx 40$$

- at $v_{e\|} \approx 3.7 v_{th}$ and thermal $v_{e\perp}$:

$$\exp\left(-\frac{m_e v^2}{2T_e}\right) \approx 4\times 10^{-4}$$

- Fraction of heat-carrying electrons (estimate based on Braginski's $\chi_{e\|}$, $v_{e\|} = 3.7 v_{th}$, $v_{e\perp\|} = v_{th}$ and $\Delta v_{\|} = v_{th}$): 1/3000



Contributions of electrons with different velocities v to the heat flux q_e

F ~400x200 mesh in velocity space is required to adequately resolve f_e-function in the region of heat-carrying electrons with $v \sim 4v_{th} \rightarrow$ 80000 equations for an implicit scheme $\Rightarrow$ large CPU time consumption.
For spatially varying T_e (e.g. from 100 eV to 1 eV) this number will rise further.

Chapman-Enskog explansion for $q_{e\|}$

$$q_{e\|} = K\frac{\partial T_e}{\partial x}\left[1+\delta_1\left(\frac{\lambda_e}{2T_e}\frac{\partial T_e}{\partial x}\right)^2+\delta_2\left(\frac{\lambda_e^2}{4T_e^2}\frac{\partial^2 T_e}{\partial x^2}\right)+\delta_3\left(\frac{\lambda_e}{2T_e}\right)^2\left(\frac{\partial T_e}{\partial x}\right)^{-1}\frac{\partial^3 T_e}{\partial x^3}\right]$$

$$\delta_1 = [7.8(Z+1)+13.1]\times 10^3$$

$$\delta_2 = [4.88(Z+1)+7.74]\times 10^3$$

$$\delta_3 = [0.3(Z+1)+0.45]\times 10^3$$

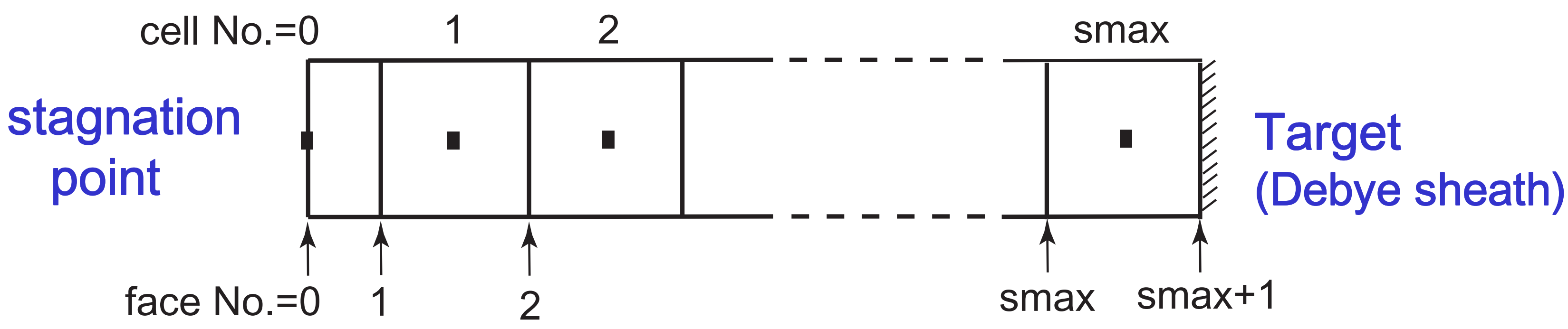
[*Luciani & Mora* (1986)]

- Large values of δ-coefficients imply significant deviations from the linear law: $q_{e\|} \propto \nabla_{\|} T_e$, already at rather modest ratios $L_{\|}/\lambda_e$ ~ 100

1d2v calculations (variation along field line)

Simple test problem:

- 1d in real space; linear geometry, from stagnation point to target plate, where Debye sheath is formed
- 2d in velocity space - full Coulomb coll. operator
- plasma ambipolarity maintained by adjusting $E_{||}$
- ion density/temperature constant along $s_{||}$ $\rightarrow$ "cold electron injection" at target in lieu of ion target sink, in order to create $\nabla_{||}T_e$



1d2v calculations: numerical scheme

- Operator splitting scheme used to solve 1d2v problem, following Shoucri & Gagne (1978) (also used by Batishchev et al.):

  - ½ Δt free-streaming
  - 1 Δt Coulomb collisions + $E_{||}$ -field force to kill momentum
  - ½ Δt free-streaming

- for the free-streaming, explicit 2nd order schemes with upwinding are being tested

ASDEX Upgrade

Preliminary results on parallel heat conduction

IPP

- Braginski heat conduction coeff. is obtained for very high collisionalities: very long systems, $s_{||} \sim 1000\,\lambda_{ei}$, are to be modelled, with T_e drop by ~ 10% $\rightarrow$ very slow profile evolution

- $\chi_{e||}$ was found to depend on Δt $\rightarrow$ long run times required due to smallness of Δt ($<< \tau_{ei}$)

Scheme implementation & CPU consumption

- Presently running on up to 64 processors on Linux cluster of IPP Garching. parallelisation using MPI. Number of spatial positions along field line: 63

- Processor No.0 (host) handles all operations for all spatial cells, except for Coulomb collisions (to be sped up in future by sharing also the free-streaming among processors)

- Coulomb collisions take large fraction of CPU time $\Rightarrow$ one proc. $\rightarrow$ one spatial pos. Time mostly consumed by:
  - Solving Fokker-Planck equation
  - 2 Poisson's equations for Rosenbluth potentials (2 potentials)
  - Specifying boundary conditions for Poisson's equations (involves large array multiplications and summations)
  - sparse matrix sover MUMPS (MUltifrontal Massively Parallel sparce direct Solver) is used 3 times for each time step

- 1 time step, when running on 64 processors, for velocity grid 200x400 takes $\approx$ 3 sec

Summary and outlook

- Basic tests/benchmarks have almost been completed: good results.
- Planning to start coupling it with SOLPS, beginning with simplest 1D geometry, for regimes with moderate T_e drop from upstream to target; coupling algorithm has yet to be developed